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Variational study of ^{3}He-^{4}He mixtures

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The ground-state properties of the ^{3}He-^{4}He mixture are investigated by assuming the wave function to be a product of pair correlations. The antisymmetry of the ^{3}He component is taken into account by Fermi-hypernetted-chain techniques and the results are compared with those obtained from the lowest-order Wu-Feenberg expansion and the boson-boson approximation. A little improvement is found in the ^{3}He maximum solubility. A microscopic theory to calculate ^{3}He static properties such as zero-concentration chemical potential and excess-volume parameter is derived and the results are compared with the experiments.

I. INTRODUCTION

Recently, there has been a renewed interest in the theoretical description of isotopic boson-fermion mixtures, mainly due to the discovering of an incomplete phase separation at $T=0$ K in ^{3}He-^{4}He mixtures.[1-3] The maximum solubility of ^{3}He in ^{4}He has been measured to be about 6.5%. Different microscopic approaches to this problem have been used in the past years[4-7] starting from a description of the system that does not incorporate the fermionic character of ^{3}He; however, this incorrect treatment of the ^{3}He symmetry properties did not allow these theories to reproduce the phase mixing. Hansen and Schiff[8] and, more recently, Guyer and Miller[9] have in fact shown that in order to obtain miscibility in the ground state of the ^{3}He-^{4}He mixtures, the presence of the Fermi-Dirac statistics in ^{3}He is necessary. In their procedure, a Slater-Jastrow wave function was used and the antisymmetrization of the ^{3}He wave function was introduced by means of a lowest-order Wu-Feenberg expansion[10] mixed to a hypernetted-chain (HNC) expansion of the bosonic component.

In this paper we have generalized the Fermi-HNC (FHNC) and HNC equations[11] to the case of a binary fermion-boson system and we have applied them to the ^{3}He-^{4}He mixtures to account for, in a more complete way, the antisymmetry of the ^{3}He wave function. Two other quantities of experimental interest and which are useful to test the microscopic models are the ^{3}He chemical potential e_1 and the excess volume parameter α_0. The first, at zero concentration of ^{3}He and zero pressure and temperature, is identical to the binding energy of one ^{3}He atom in ^{4}He, and its experimental value is -2.795 K. The presence of an excess-volume parameter is a consequence of the fact that the ^{3}He particle has a larger zero-point energy than the ^{4}He because of the lighter mass and therefore has a larger specific volume. The α_0 experimental value is 0.284. Woo, Massey, and Tan[4] (WMT) have developed a microscopic theory that involves the knowledge of the radial distribution functions of a binary boson system to calculate α_0 and e_1.

Here we present the formulas for the radial distribution functions, in an HNC approach, of a boson system with two internal impurities; then the WMT theory of calculating the ^{3}He chemical potential and α_0 is applied. The plan of the paper is the following. In Sec. II the generalization of the FHNC and HNC equations to fermion-boson mixtures and the energy equations are derived; in Sec. III the expansion to calculate e_1 and α_0 is presented; in Sec. IV the results are presented and a brief discussion of them is made; finally, the last section contains a brief conclusion.

II. FHNC-HNC EQUATIONS FOR ^{3}He-^{4}He MIXTURES

We consider a homogeneous, isotopic mixture compound of N_3 ^{3}He atoms and N_4 ^{4}He atoms, confined in a box of volume Ω with densities $\rho_3=N_3/\Omega$ and $\rho_4=N_4/\Omega$ and $\rho=\rho_3+\rho_4$ and concentrations $x_3=N_3/(N_3+N_4)$ and $x_4=N_4/(N_3+N_4)$; at the end we let N_3, N_4, and Ω go to ∞, keeping the densities constant. The Hamiltonian of such a system is

$$H=-\frac{\hbar^2}{2m_4}\sum_{i=1}^{N_4}\nabla_i^2-\frac{\hbar^2}{2m_3}\sum_{i=1}^{N_3}\nabla_i^2+\sum_{\substack{i=1\\i<j}}^{N_4}V^{(4,4)}(i,j)+\sum_{\substack{i=1\\i<j}}^{N_3}V^{(3,3)}(i,j)+\sum_{i=1}^{N_4}\sum_{j=1}^{N_3}V^{(4,3)}(i,j)\ , \tag{2.1}$$

where $V^{(\alpha,\beta)}$ are the interaction potentials between the particles of the α and β types, repulsive at short distances (here and in the following we will use Greek indices to stand for 3 and 4). To describe the system we adopt a variational choice and simple generalization of the Jastrow wave function used to describe the separate components; then

$$\psi(1,\ldots,N_4,N_{4+1},\ldots,N_3+N_4)=\left[\prod_{\substack{i=1\\i<j}}^{N_3}f^{(3,3)}(i,j)\right]\left[\prod_{\substack{i=1\\i<j}}^{N_4}f^{(4,4)}(i,j)\right]\left[\prod_{i=1}^{N_4}\prod_{j=1}^{N_3}f^{(4,3)}(i,j)\right]\times\phi(1,\ldots,N_3)\ , \tag{2.2}$$

where $f^{(\alpha,\beta)}(i,j)$'s are the correlation functions between the i α particle and the j β particle, with the usual boundary conditions

$$\lim_{r_{ij}\to 0}f^{(\alpha,\beta)}(i,j)=0,\quad \lim_{r_{ij}\to\infty}f^{(\alpha,\beta)}(i,j)=1\ , \tag{2.3}$$

and $\phi(1,\ldots,N_3)$ is the Slater determinant of plane waves relative to the Fermi component of the mixture.

We are mainly interested in the calculation of the ground-state energy, so it is useful to consider the α-β radial distribution functions:

$$g^{(\alpha,\beta)}(r_{ij})=\frac{N_\alpha(N_\beta-\delta_{\alpha\beta})}{\rho_\alpha\rho_\beta}\frac{\int|\psi|^2d\Omega(i,j)}{\mathcal{I}}\ , \tag{2.4}$$

with $\mathcal{I}$ the normalization integral and where $d\Omega(i,j)$ indicates the integration over all the particle coordinates except i and j ($i\in\{\alpha\}$ and $j\in\{\beta\}$). Now, we will derive the $g^{(\alpha,\beta)}$'s generalizing the HNC and FHNC techniques to a binary system. To make this, we need to construct the sets of all the possible nodal and non-nodal diagrams (we will work in HNC/0 and FHNC/0 approximation, i.e., we will disregard all the contributions coming from the elementary, or bridge, diagrams) and to calculate the functions corresponding to their sums.

The functions are denoted as $N_{dd}^{(\alpha,\beta)}$, $N_{de}^{(\alpha,3)}$, $N_{ee}^{(3,3)}$, and $N_{cc}^{(3,3)}$ and $X_{dd}^{(\alpha,\beta)}$, $X_{de}^{(\alpha,3)}$, $X_{ee}^{(3,3)}$, and $X_{cc}^{(3,3)}$. The first set of functions refers to the sums of the nodal diagrams and the second to the non-nodal ones. The subscripts indicate the types of correlation lines reaching the external points (d denotes direct, e denotes exchange, and c denotes cyclic) and the superscripts the types of particles (^{3}He or ^{4}He) at the same points. These functions are the solutions of the following seven integral equations:

$$\begin{aligned}
N_{dd}^{(\alpha,\beta)}&=\sum_{\lambda=3,4}\rho_\lambda(X_{dd}^{(\alpha,\lambda)}\,|\,X_{dd}^{(\lambda,\beta)}+N_{dd}^{(\lambda,\beta)})+\rho_3(X_{de}^{(\alpha,3)}\,|\,X_{dd}^{(3,\beta)}+N_{dd}^{(3,\beta)})+\rho_3(X_{dd}^{(\alpha,3)}\,|\,X_{ed}^{(3,\beta)}+N_{ed}^{(3,\beta)})\ ,\\
N_{de}^{(\alpha,3)}&=\sum_{\lambda=3,4}\rho_\lambda(X_{dd}^{(\alpha,\lambda)}\,|\,X_{de}^{(\lambda,3)}+N_{de}^{(\lambda,3)})+\rho_3(X_{de}^{(\alpha,3)}\,|\,X_{de}^{(3,3)}+N_{de}^{(3,3)})+\rho_3(X_{dd}^{(\alpha,3)}\,|\,X_{ee}^{(3,3)}+N_{ee}^{(3,3)})\ ,\\
N_{ee}^{(3,3)}&=\sum_{\lambda=3,4}\rho_\lambda(X_{ed}^{(3,\lambda)}\,|\,X_{de}^{(\lambda,3)}+N_{de}^{(\lambda,3)})+\rho_3(X_{ee}^{(3,3)}\,|\,X_{de}^{(3,3)}+N_{de}^{(3,3)})+\rho_3(X_{ed}^{(3,3)}\,|\,X_{ee}^{(3,3)}+N_{ee}^{(3,3)})\ ,\\
N_{cc}^{(3,3)}&=\rho_3[X_{cc}^{(3,3)}\,|\,X_{cc}^{(3,3)}+N_{cc}^{(3,3)}-\ell(k_Fr)/\nu]\ ,
\end{aligned} \tag{2.5}$$

where $\ell(x)=3(\sin x-x\cos)/x^3$, $k_F=6\pi^2\rho_3/\nu$, and ν is the degeneracy of the Fermi component. The convolution integral is defined as follows:

$$(f^{(\alpha,\beta)}\,|\,g^{(\beta,\gamma)})=\int d\bar{r}_3f^{(\alpha,\beta)}(r_{13})g^{(\beta,\gamma)}(r_{32})\ . \tag{2.6}$$

The non-nodal functions are

$$\begin{aligned}
X_{dd}^{(\alpha,\beta)}(r)&=(f^{(\alpha,\beta)}(r))^2 e^{N_{dd}^{(\alpha,\beta)}(r)}-1-N_{dd}^{(\alpha,\beta)}(r)\ ,\\
X_{de}^{(\alpha,3)}(r)&=[(f^{(\alpha,3)}(r))^2 e^{N_{dd}^{(\alpha,3)}(r)}-1]N_{de}^{(\alpha,3)}(r)\ ,\\
X_{ee}^{(3,3)}(r)&=(f^{(3,3)}(r))^2 e^{N_{dd}^{(3,3)}(r)}\{N_{ee}^{(3,3)}(r)+(N_{de}^{(3,3)}(r))^2-\nu[\ell(k_Fr)/\nu+N_{cc}^{(3,3)}(r)]^2\}-N_{ee}^{(3,3)}(r)\ ,\\
X_{cc}^{(3,3)}(r)&=[(f^{(3,3)}(r))^2 e^{N_{dd}^{(3,3)}(r)}-1][N_{cc}^{(3,3)}(r)-\ell(k_Fr)/\nu]\ .
\end{aligned} \tag{2.7}$$

By means of these functions we can write the radial distribution functions

$$g^{(4,4)}(r)=1+N_{dd}^{(4,4)}(r)+X_{dd}^{(4,4)}(r)\ , \tag{2.8a}$$

$$g^{(4,3)}(r)=1+N_{dd}^{(4,3)}(r)+X_{dd}^{(4,3)}(r)+N_{de}^{(4,3)}(r)+X_{de}^{(4,3)}(r)\ , \tag{2.8b}$$

$$g^{(3,3)}(r)=1+N_{dd}^{(3,3)}(r)+X_{dd}^{(3,3)}(r)+N_{ee}^{(3,3)}(r)+X_{ee}^{(3,3)}(r)+2[N_{de}^{(3,3)}(r)+X_{de}^{(3,3)}(r)]\ . \tag{2.8c}$$

The boson-boson approximation is obtained by putting zero $N_{ij}^{(\alpha,\beta)}$ and $X_{ij}^{(\alpha,\beta)}$ for (i,j) different from (d,d) in Eqs. (2.5) and (2.7). So we have in this approximation

$$g_{BB}^{(\alpha,\beta)}(r)=1+N_{dd}^{(\alpha,\beta)}(r)+X_{dd}^{(\alpha,\beta)}(r) \tag{2.9}$$

for $\alpha,\beta=3,4$. At the lowest order of the Wu-Feenberg expansion the radial distribution function of the ^{3}He component is given by

$$g_{\rm WF}^{(3,3)}(r)=g_{BB}^{(3,3)}(r)[1-\ell^2(k_Fr)/\nu]\ . \tag{2.10}$$

The energy per particle of the binary system is

$$\frac{E}{N}=x_BE^{(4)}(\rho_3,\rho_4)+x_FE^{(3)}(\rho_3,\rho_4)+x_Bx_FE^{(m)}(\rho_3,\rho_4)\ , \tag{2.11}$$

where $E^{(3)}$ and $E^{(4)}$ represent the energies of the fermionic ^{3}He and of the bosonic ^{4}He components and $E^{(m)}$ is the energy coming from their interaction; using the Fantoni-Rosati[12] form of the kinetic energy for a Fermi system, the various parts of Eq. (2.11) may be written as

$$\begin{aligned}
E^{(4)}&=\frac{\rho_4}{2}\int d\bar{r}\,g^{(4,4)}(r)\left[V^{(4,4)}(r)-\frac{\hbar^2}{2m_4}\nabla^2\ln f^{(4,4)}(r)\right]\ ,\\
E^{(m)}&=\rho\int d\bar{r}\,g^{(4,3)}(r)\left[V^{(4,3)}(r)-\frac{\hbar^2}{2\mu}\nabla^2\ln f^{(4,3)}(r)\right]\ ,\\
E^{(3)}&=\frac{\rho_3}{2}\int d\bar{r}\,g^{(3,3)}(r)\left[V^{(3,3)}(r)-\frac{\hbar^2}{2m_3}\nabla^2\ln f^{(3,3)}(r)\right]+T^{(1)}(\rho_3)+T^{(2)}(\rho_3)+T^{(3)}(\rho_3)\ ,
\end{aligned} \tag{2.12}$$

where $T^{(1)}=\frac{3}{10}\hbar^2k_F^2/m_3$ and $T^{(2)}$ and $T^{(3)}$ are the two- and three-body terms of the kinetic energy obtained from the application of the derivative operator to the Slater determinant.[12] The reduced mass μ is

$$\frac{1}{\mu}=\frac{1}{2}\left[\frac{1}{m_3}+\frac{1}{m_4}\right]\ . \tag{2.13}$$

In the boson-boson approximation we have $T^{(i)}=0$ for $i=1,2,3$ while in the WF approximation $T^{(1)}$ is the same as in FHNC, $T^{(3)}=0$ and

$$T_{\rm WF}^{(2)}=-\frac{\hbar^2}{8m_3}\rho_3\int d\bar{r}\,g_{BB}^{(3,3)}(r)\frac{\nabla^2l^2(k_Fr)}{\nu}\ . \tag{2.14}$$

In terms of the energy and of the pressure

$$P=\rho^2\left[\frac{\partial E}{\partial\rho}\right]_{x_3}\ ,$$

we can calculate the enthalpy per particle,

$$H(x_3,P)=\frac{E(x_3,\rho)}{N}+\frac{P(x_3,\rho)}{\rho} \tag{2.15}$$

and the chemical potential of the α component,

$$\mu_\alpha = H + x_\beta \left[\frac{\partial H}{\partial x_\alpha} \right]_P . \tag{2.16}$$

These two quantities give direct information about the phase behavior of the mixture.[3]

III. HNC CALCULATION OF THE ^{3}He STATIC PROPERTIES

In the WMT theory,[4] the expectation value of the Hamiltonian (2.1) for a binary boson system was written as

$$\langle H \rangle = N_4 E_0(\rho_4) + N_3 E_1(\rho_4) + \frac{N_3^2}{N_4} E_2(\rho_3,\rho_4) , \tag{3.1}$$

where $E_0(\rho_4)$ is the energy per particle of pure ^{4}He at density ρ_4, $E_1(\rho_4)$ is the chemical potential of one ^{3}He atom in ^{4}He at that density and $E_2(\rho_3,\rho_4)$ may be interpreted as an interaction term between the mass-3 bosons. A different form of $\langle H \rangle$ is the following:

$$\langle H \rangle = N_4 e_0(\rho_4) + N_3 e_1(\rho_4) + \frac{N_3^2}{N_4} e_2(\rho_4) + O\left[\frac{N_3^3}{N_4^2} \right] . \tag{3.2}$$

The first two terms of formulas (3.1) and (3.2) are the same ($e_0 = E_0$ and $e_1 = E_1$); e_2 is the energy of a system compound from N_4 ^{4}He atoms plus two ^{3}He impurities of opposite spins. It is clear that

$$E_2(\rho_3,\rho_4) = e_2(\rho_4) + O\left[\frac{N_3}{N_4} \right] . \tag{3.3}$$

In the zero concentration limit ($x_3 \rightarrow 0$) we have $e_2 = E_2$. Using Eq. (2.2) with $\phi = 1$ the explicit expression for the e_i's are

$$e_0(\rho_4) = \frac{\rho_4}{2} \int d\bar{r}\, g_0^{(4,4)}(r) \left[V^{(4,4)}(r) - \frac{\hbar^2}{2m_4} \nabla^2 \ln f^{(4,4)}(r) \right] , \tag{3.4a}$$

$$\begin{aligned} e_1(\rho_4) = {} & \frac{\rho_4}{2} \int d\bar{r}\, g_0^{(4,3)}(r) \left[2V^{(4,3)}(r) - \frac{\hbar^2}{2\mu} \nabla^2 \ln f^{(4,3)}(r) \right] \\ & + \frac{\rho_4^2}{2} \int d\bar{r}\, g_1^{(4,4)}(r) \left[V^{(4,4)}(r) - \frac{\hbar^2}{2m_4} \nabla^2 \ln f^{(4,4)}(r) \right] , \end{aligned} \tag{3.4b}$$

$$\begin{aligned} e_2(\rho_4) = {} & \frac{\rho_4}{2} \int d\bar{r}\, g_0^{(3,3)}(r) \left[V^{(3,3)}(r) - \frac{\hbar^2}{2m_3} \nabla^2 \ln f^{(3,3)}(r) \right] \\ & + \frac{\rho_4^2}{2} \int d\bar{r}\, g_1^{(4,3)}(r) \left[2V^{(4,3)}(r) - \frac{\hbar^2}{2\mu} \nabla^2 \ln f^{(4,3)}(r) \right] \\ & + \frac{\rho_4^3}{2} \int d\bar{r}\, g_2^{(4,4)}(r) \left[V^{(4,4)}(r) - \frac{\hbar^2}{2m_4} \nabla^2 \ln f^{(4,4)}(r) \right] , \end{aligned} \tag{3.4c}$$

$g_n^{(\alpha,\beta)}(r)$ is the radial distribution function of the α-β type with n internal impurities (^{3}He atoms).

In the HNC/0 approximation the distribution functions $g_0^{(\alpha,\beta)}$'s are easily obtained from the solutions of the following set of equations:

$$N_0^{(\alpha,\beta)}(r) = \rho_4 (X_0^{(\alpha,4)} \mid X_0^{(4,\beta)} + N_0^{(4,\beta)}) , \tag{3.5a}$$

$$X_0^{(\alpha,\beta)}(r) = (f^{(\alpha,\beta)}(r))^2 e^{N_0^{(\alpha,\beta)}(r)} - 1 - N_0^{(\alpha,\beta)}(r) , \tag{3.5b}$$

and

$$g_0^{(\alpha,\beta)}(r) = 1 + N_0^{(\alpha,\beta)}(r) + X_0^{(\alpha,\beta)}(r) . \tag{3.5c}$$

The $g_1^{(4,\beta)}$'s are defined as

$$g_1^{(4,\beta)}(r) = g_0^{(4,\beta)}(r) [N_{1'}^{(4,\beta)}(r) + N_1^{(4,\beta)}(r)] , \tag{3.6a}$$

where

$$N_{1'}^{(4,\beta)}(r)=(g_0^{(4,3)}-1\,|\,g_0^{(3,\beta)}-1) \tag{3.6b}$$

is the sum of the nodal diagrams of 4-β type with one ^{3}He impurity on a node, and

$$N_1^{(4,4)}(r)=2\rho_4(g_0^{(4,4)}-1\,|\,X_1^{(4,4)})+\rho_4(g_0^{(4,4)}-1\,|\,\rho_4(X_1^{(4,4)}\,|\,g_0^{(4,4)}-1))\ , \tag{3.6c}$$

$$N_1^{(4,3)}(r)=\rho_4(g_0^{(4,4)}-1\,|\,X_1^{(4,3)})+\rho_4(X_1^{(4,4)}\,|\,g_0^{(4,3)}-1)+\rho_4(g_0^{(4,4)}-1\,|\,\rho_4(X_1^{(4,4)}\,|\,g_0^{(4,3)}-1))\ , \tag{3.6d}$$

with

$$X_1^{(4,\alpha)}(r)=g_1^{(4,\alpha)}(r)-N_1^{(4,\alpha)}(r)-N_{1'}^{(4,\alpha)}(r)\ . \tag{3.6e}$$

Finally, for $g_2^{(4,4)}(r)$ we have

$$g_2^{(4,4)}(r)=g_0^{(4,4)}(r)\{\,N_2^{(4,4)}(r)+N_{2'}^{(4,4)}(r)+[N_1^{(4,4)}(r)+N_{1'}^{(4,4)}(r)]^2\,\}\ , \tag{3.7a}$$

where

$$N_{2'}^{(4,4)}(r)=(g_0^{(4,3)}-1\,|\,g_1^{(3,4)}) \tag{3.7b}$$

is the sum of all the nodal diagrams of the 4-4 type with two ^{3}He impurities on the internal points and at least one of them on a node, and $N_2^{(4,4)}(r)$ is the solution of the following integral equation:

$$\begin{aligned}N_2^{(4,4)}(r)= {} & 2\rho_4(g_0^{(4,4)}-1\,|\,X_2^{(4,4)})+\rho_4(g_0^{(4,4)}-1\,|\,\rho_4(X_2^{(4,4)}\,|\,g_0^{(4,4)}-1))\\ &+\rho_4(X_1^{(4,4)}\,|\,X_1^{(4,4)}+N_1^{(4,4)})+\rho_4(g_0^{(4,4)}-1\,|\,\rho_4(X_1^{(4,4)}\,|\,\rho_4(X_1^{(4,4)}\,|\,X_1^{(4,4)}+N_1^{(4,4)}))\ ,\end{aligned} \tag{3.7c}$$

with

$$X_2^{(4,4)}(r)=g_2^{(4,4)}(r)-N_2^{(4,4)}(r)-N_{2'}^{(4,4)}(r)\ . \tag{3.7d}$$

In the WMT theory, the knowledge of E_0, E_1, and E_2 allows the calculation of the static properties of ^{3}He in ^{4}He; applying these results at zero concentration, we can write

$$\left[\frac{\partial e_1}{\partial \rho_4}\right]=(1+\alpha_0)\frac{m_4 s^2}{\rho_4} \tag{3.8}$$

and

$$2e_2(\rho_4)=(1+2\alpha_0)m_4 s^2\ , \tag{3.9}$$

where s is the sound velocity in pure ^{4}He at that density.

IV. RESULTS

As a starting point of this section, we discuss the energy properties and the phase behavior of liquid ^{3}He-^{4}He mixtures at zero Kelvin temperature and zero atmosphere pressure. In these conditions, the energy per particle is identical to the enthalpy per particle. It has to be noted that our zero pressure comes from the FHNC-HNC approximation and the corresponding equilibrium density is well far from the experimental one.

We assume that the $V^{(\alpha,\beta)}$ interactions appearing in the Hamiltonian (2.1) are all of the form

$$V(r)=4\epsilon\left[\left[\frac{\sigma}{r}\right]^{12}-\left[\frac{\sigma}{r}\right]^{6}\right] \tag{4.1}$$

with $\epsilon=10.22$ K and $\sigma=2.556$ Å; the correlation factors between the α-type and β-type particles are taken identical for all the pairs and of the commonly used short-range form

$$f(r)=\exp\left[-\left[\frac{b\sigma}{r}\right]^{5}\frac{1}{2}\right] \tag{4.2}$$

with b as unique variational parameter.

In order to study the energy of the ground state of the mixture for different ^{3}He concentrations, we fix x_3 and then perform a minimization respect to b and the density. This, together with the condition $\rho^2(\partial E/\partial\rho)=0$, determines the total equilibrium density for a given x_3 and ensures us to have zero pressure.

The excess energy per particle E_{ex} is related to the heat that must be removed or added to the system in order to keep constant the temperature and is defined as

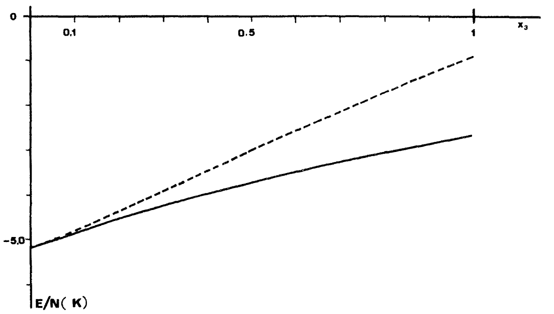

FIG. 1. E/N results. —boson-boson approximation; – – – FHNC-HNC approximation.

$$E_{\rm ex}(x_3)=E(x_3)-(1-x_3)E(0)-x_3E(1) \ , \tag{4.3}$$

where all the quantities are evaluated at zero pressure and temperature. When we study the energy diagram, looking for regions of instability requires $d^2E/dx_3^2<0$ or, in an equivalent way, $d^2E_{\rm ex}/dx_3^2<0$. When this condition occurs, the system is completely unstable against phase separation. The condition $d^2E/dx_3^2=0$ gives the frontier of the region with the absolutely unstable systems and determines the spinoidal concentration x_3^s; the maximum solubility concentration x_3^m lies a little bit before and is fixed from the condition of the equality of the ^{3}He chemical potential in pure phase with that in the mixed one:

$$\mu_3(x_3^m)=\mu_3(1) \ . \tag{4.4}$$

We can rewrite this condition in terms of $E_{\rm ex}$,

$$E_{\rm ex}(x_3)+(1-x_3)\frac{dE_{\rm ex}(x_3)}{dx_3}=0 \ . \tag{4.5}$$

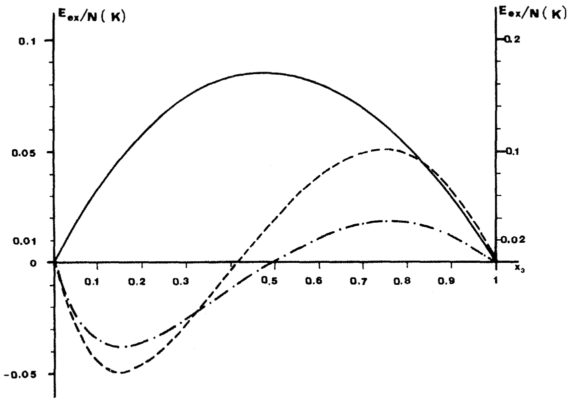

FIG. 2. $E_{\rm ex}/N$ results. — boson-boson approximation; – – – FHNC-HNC approximation; —·—·—· lowest-order Wu-Feenberg approximation. The right scale refers only to the boson-boson values.

TABLE I. Calculated values of the maximum ^{3}He solubility x_3^m and of the spinoidal concentration x_3^s. *BB*, boson-boson; WF, lowest-order Wu-Feenberg approximation; FH, FHNC-HNC approximation, expt., experimental results.

	BB	WF	FH	Expt.
x_3^m	0	0.18	0.16	0.064
x_3^s	0	0.38	0.39	0.15

The region between the two concentrations x_3^s and x_3^m is the locus of the metastable concentrations.

In Figs. 1 and 2 we present the values of E and $E_{\rm ex}$ obtained by using the following different approximations.

(a) Boson-boson: We consider only the underlying boson-boson system without taking care of the antisymmetrization of the ^{3}He [Eq. (2.9)].

(b) Wu-Feenberg at lowest order: As in Ref. 9, the antisymmetrization is properly included only at lowest order [Eq. (2.10)].

(c) FHNC-HNC: All the effects of the antisymmetry are considered except those contained in the elementary diagrams [Eq. (2.8)].

In Table I the results for x_3^m and x_3^s in the different approximations are reported. As it has been already established,[7,9] the boson-boson solution is completely unstable and no mixture at all takes place. The differences between the other two calculations are not large and, in spite of the small improvement of the FHNC-HNC results, we are still far from the experimental values.

Of course, to calculate $E_{\rm ex}$ requires much more attention than to calculate the energies of the single pure components, because the first quantity is 2 orders of magnitude smaller, and therefore the evaluation of the derivatives is a very delicate task. Our feeling is that the calculations (performed by us) are accurate enough. The differences from the experimental results are not percentually larger than those in the pure phases. In this respect, we think that even the inclusion of the omitted diagrams will not improve significantly the conclusions (for pure ^{3}He the elementary diagrams' contribution to the energy[13] is about 10%). Similarly, an optimal correlation factor, coming from the solution of the Euler equation for the FHNC-HNC energy, would not considerably improve the description of the system.[14–16]

We think that the main source of disagreement between the calculated x_3^m and its experimental value is the large error ($E_{\rm FHNC}=-0.92$ K) in the

TABLE II. Calculated values of the zero-concentration chemical potential e_1 and of the excess-volume parameter α_0 for ^{3}He. M denotes microscopic and A denotes analytical calculations; expt., experimental values.

	M	A	Expt.
e_1 (K)	-1.89	-1.90	-2.79
α_0	0.38	0.31	0.28

estimation of the pure ^{3}He energy. Because of this, the system is energetically favorited in the mixed phase; in fact, to get mixing, it is also essential that the ^{3}He chemical potential at zero concentration be smaller than that in the pure phase, but as the experimental difference between them is smaller than that calculated with the FHNC-HNC results, we have a larger x_3^m.

In Table II we present different results for the zero-concentration chemical potential of ^{3}He (e_1) at zero pressure and for the excess-volume parameter α_0. The values under the M column (microscopic) are derived from the equations of the Sec. III of this paper; those under the A column (analytic) come directly from the curves of Figs. 1 and 2 employing the formula

$$\alpha_0 = \lim_{x_3 \to 0} \frac{\rho(x_3) - \rho_4}{x_3 \rho_4} , \tag{4.6}$$

where $\rho(x_3)$ is the equilibrium density of the mixture at the x_3 concentration of ^{3}He and ρ_4 is the equilibrium density of pure ^{4}He, and

$$e_1 = \mu_3(x_3 = 0) = E(0) + \left[\frac{\partial E}{\partial x_3} \right]_{x_3 = 0, P} . \tag{4.7}$$

In the expt. column the experimental values are reported. The agreement between the two calculated values of e_1 is very good. This fact is a strong indication of the accuracy of the two procedures. The values of α_0 are also in good agreement if we have present that numerical derivatives are necessary in order to obtain them. The comparison with respect to the experimental results shows a percentual error not larger than that made in the pure phase calculations. We realize that this type of wave function allows a better description of the ^{3}He-^{4}He system at very low concentrations of ^{3}He. This is in accordance with the fact that the simple Jastrow wave function gives a disagreement of about 25% in the ground-state energy estimation for pure ^{4}He and 60% for pure ^{3}He.

We have also made calculations with different parameters for every type of pairs in the two-body correlation function, but the results are not significantly affected. We think that effective improvements can be achieved by introducing effective three-body correlation in the wave function and momentum dependence. This conclusion is strongly supported from the results in the estimation of the energy of the pure phases[17] and of the ^{3}He effective mass[14] with this more complete wave function.

V. CONCLUSIONS

The FHNC-HNC theory has been generalized to apply for boson-fermion mixtures and specifically for the description of the ^{3}He-^{4}He system. The system is as well described as in the pure phases. As was expected, the disagreement between the simpler lowest-order Wu-Feenberg approximation and the FHNC-HNC approach increases with the ^{3}He concentration and a small improvement is obtained in the calculated value of the ^{3}He maximum solubility.

The ^{3}He static properties at very low concentrations, chemical potential, and excess-volume parameter are better reproduced than the pure ^{3}He energy. At low concentrations, the mean distance between the ^{3}He atoms is large compared to that in the pure phase, and the effective interaction between two of them does not depend too much on the Fermi-Dirac statistics, but in order to obtain good agreement with the experimental values it is necessary to improve the description of the mixing by introducing a more complete wave function than the simple Jastrow-Slater employed in this paper.

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